Nuclear Masses for Simulation Databases

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Nuclear masses determine the energy balance in nuclear reactions. For example, in radioactive decay such as α and β decay, in element synthesis reactions such as neutron capture in stars, and in heavy-ion reactions in laboratories. In a nuclear reactor, power is generated when uranium fissions into two fragments. Many different mass and charge splits may occur, leading to hundreds of different isotopes of about 40 different elements. To understand the properties of a reactor, a model of these decays is needed. The energy released in, and the half-life of a decay from a parent nucleus to one or more daughters are governed by the relative masses of the parent and daughter(s). Some of the masses involved have been measured, but many have not, due to their short lifetimes. Masses of such short-lived or hard-to-produce isotopes have to be obtained from a model. The most used nuclear mass model in the world was developed at Los Alamos. It involves calculating the shape and energy of the most stable nuclear configuration for each isotope (its ground state). The model takes microscopic effects into account by solving the quantum-mechanical Schrödinger equation on a cluster of computers, leading to masses for any proton number Z and neutron number N. A first model was published in 1981 and an improved one in 1995 [1]. A measure of the importance of this work is that it is the most downloaded paper from this journal 12 years after publication, and that the model tables are the preferred or only database for theoretical nuclear masses at, for example, the National Nuclear Data Center at Brookhaven National Laboratory and the International Atomic Energy Agency. Our paper has also been one of the three or so most cited LANL papers since its publication in 1995.

A goal for a theory of nuclear masses is that it be able to accurately predict masses of nuclei for which no measured values are available. Our finite range droplet model (FRDM) (1992), published in 1995, was adjusted to a 1989 database of nuclear masses. In 1997 we compared our published masses to 217 experimental masses measured after 1989 and found that the average error was unchanged (Fig. 1). The most recent experimental database has 529 "new" masses measured since 1989. The error of our masses with respect to the new data [2] is 0.46 MeV, much smaller than with respect to the 1989 data, (Fig. 2). An interesting observation is that some points on the proton-rich side of β stability indicating large deviations

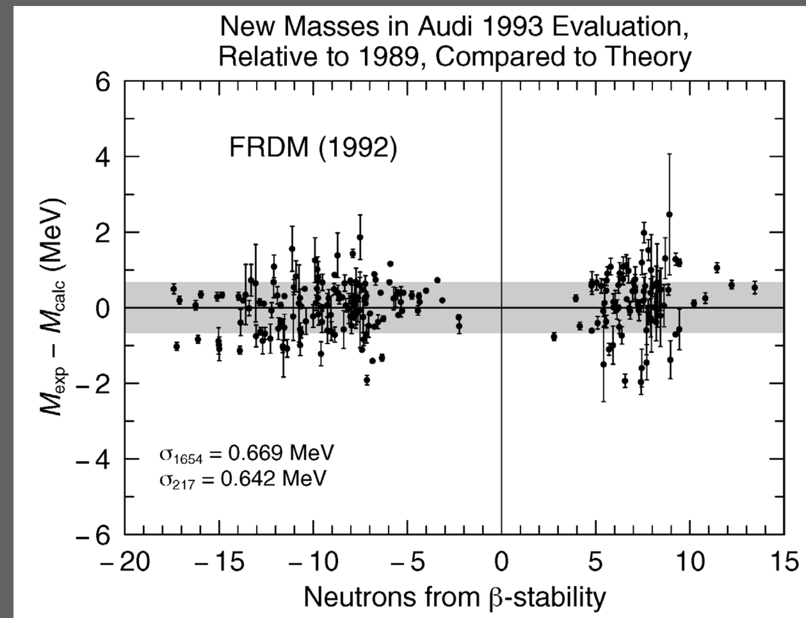

Fig. 1. Our mass model FRDM (1992) was adjusted to a 1989 database of experimental masses. We here compare the model predictions to masses measured after 1989 up to 1993. No increase in the model error is observed. The light gray area is the model one-sigma error for nuclear masses to which the model was adjusted.

between theory and experiment in Fig. 1 are not present in Fig. 2. Since the theory is unchanged, the difference means that several experimental masses were either removed from the evaluated database, or changed by more than the error bars!

Another way to study the model reliability is to plot the difference between calculated and experimental masses for each proton number Z and neutron number N. In Fig. 3, we show the differences with respect to the 1989 data to which the model was adjusted. In Fig. 4, we show the differences with respect to all the 2003 masses. Significantly, the previously unknown nuclei along the upper and lower edges of the colored region in Fig. 4 exhibit very small differences between the model and recently measured masses.

Because the computer resources available to us are 100,000 times more powerful than when we started our work on the FRDM (1992) in 1987, we have undertaken a more accurate and sophisticated determination of ground-state shapes. This work is almost completed, leading to a mass table with an average error of about 0.585 MeV (compared to the previous average error of 0.669 MeV).

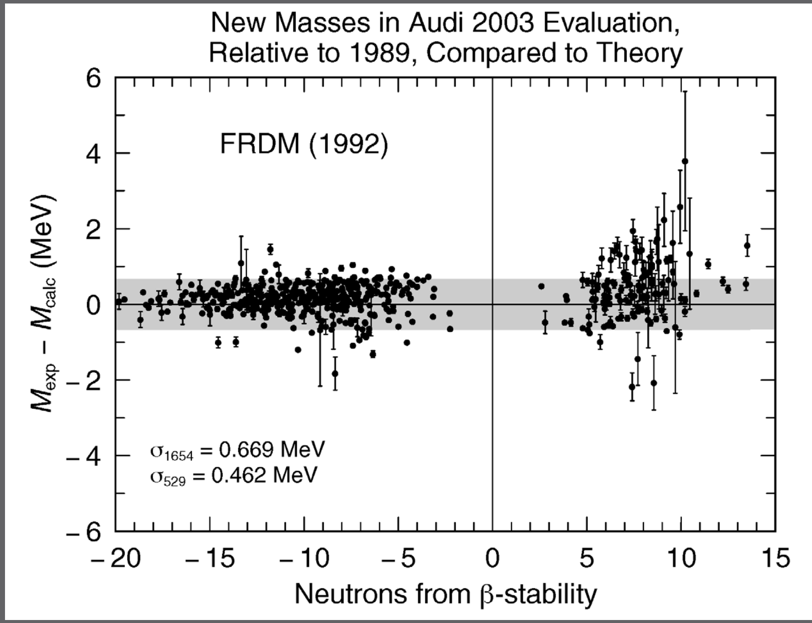

Fig. 2. Since 1993 an additional 300 masses have been measured so we can now compare our model predictions to more than 500 masses that were not known to us when the model calculations were published. The predictive power is excellent and the error for the predicted masses is considerably smaller than in the region where the model was adjusted. Moreover, masses on the proton-rich side, which in Fig. 1 exhibit some of the largest deviations from our calculated masses, are no longer present in this figure. This means they have been found in error and removed from the evaluated database, or the measured values have been revised by more than the error bars.

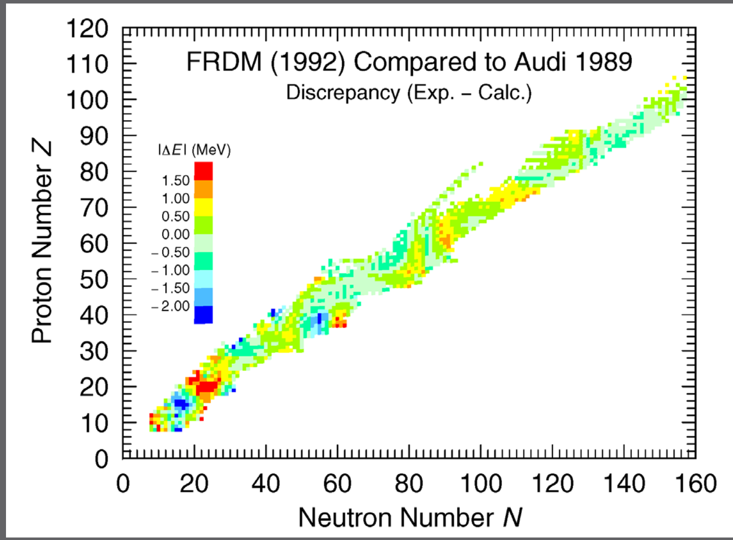

Fig. 3. Calculated masses compared to those experimental masses to which the model parameters were adjusted.

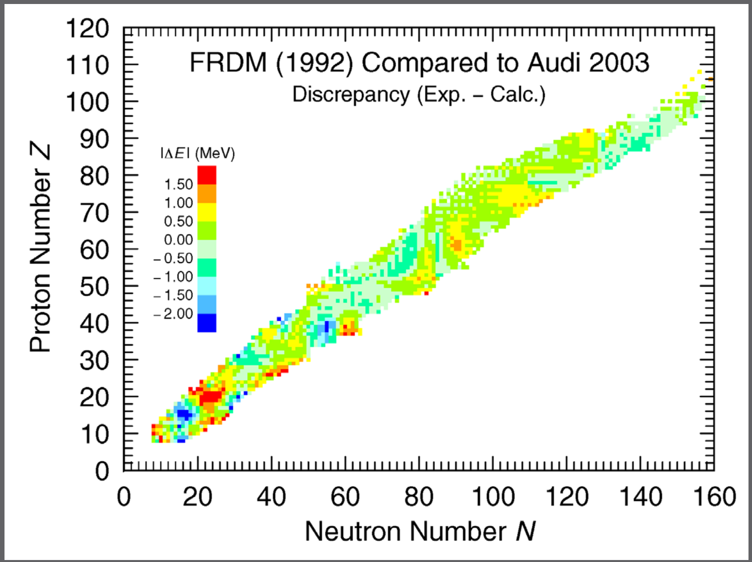

Fig. 4. Calculated masses compared to all experimental masses in the most recent evaluation. More than 500 masses were not known when the model was presented. The model gives excellent predictions of masses for these nuclei.

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[1] Atomic Data and Nuclear Data Tables **59,** 185 (1995).
[2] E. Pinheiro, W.D.Weber, and L.A. Barroso, In *Proceedings of the1995 International Conference on Parallel Processing (ICPP)* (1995).

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